Evaluation of the extraction efficiency of the QuEChERS method on incurred pesticides.

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1. Aim and scope

Validation studies are often conducted with spiked blank samples. This has the disadvantage that it deviates from the actual way pesticides are applied in the field (in many cases, by irrigation or spraying). When incurred, pesticides are incorporated into the plant system and may therefore be more difficult to extract than if spiked. This study will clarify and evaluate the extraction efficiency of incurred pesticides when using the QuEChERS extraction method. Some of the parameters evaluated will be the effect of repeated extractions with acetonitrile, and extended extraction time.

2. Short description

The analysis of pesticide residues in crops is a critical component of food safety and environmental monitoring. Traditional validation methods often rely on spiked samples to simulate pesticide contamination, yet these do not accurately represent the dynamics of pesticide behavior in real-world agricultural practices. When pesticides are applied to crops through irrigation or spraying, they are absorbed into plant tissues, leading to more complex interactions that may hinder their extraction during analysis.

Incurred pesticide residues, which are integrated into the plant's biological system, present a significant challenge for standard extraction techniques. The QuEChERS method, while effective for a wide range of pesticides, may underperform in fully extracting these tightly bound residues. This has prompted researchers to explore modifications to the extraction process, including the use of sequential extractions and longer extraction periods to enhance the recovery rates of incurred pesticides.

For this evaluation, real samples with positive detections were analyzed: 4 tomatoes, 3 spinaches, 5 bananas, 2 strawberries, 4 zucchinis, and 4 melons, resulting in a total of 22 real samples. The double extraction of the sample using the QuEChERS citrate method was evaluated. Additionally, different extraction times were assessed while the sample was in contact with the QuEChERS salts, specifically 3 minutes, 6 minutes, and 10 minutes.

3. Experimental

3.1. Sample treatment

Real samples (containing incurred pesticides) were extracted using the QuEChERS method. The general experimental procedure was as follows:

1. Weigh 10 g of sample in a 50-mL PTFE centrifuge tube.
2. Add 10 mL acetonitrile.
3. Shake the sample in an axial agitator (Agitax) for 3 minutes.
4. Add 4 g anhydrous magnesium sulphate, 1 g sodium chloride, 1 g trisodium citrate dihydrate and 0.5 g disodium hydrogencitrate sesquihydrate and shake manually (3 sec).
5. Shake the sample in an axial agitator (Agitax) for 3 minutes.

6. Centrifuge the tubes at 4000 rpm for 5 min.
7. Transfer 5 mL of the supernatant to a 15-mL PFTE centrifuge tube containing 750 mg of anhydrous magnesium sulfate and 125 PSA and vortex for 30 sec.
8. Centrifuge the tubes at 4000 rpm for 5 min.
9. Transfer the supernatant to a 4-mL vial and add 10 µL/mL of extract of ACN (5% formic acid)

In this technical report, the consecutive execution of the QuEChERS extraction method was evaluated, which was the first parameter assessed (**Figure 1**). It is important to emphasize that for quantification of the extracts, a blank that had undergone the same sample treatment was employed.

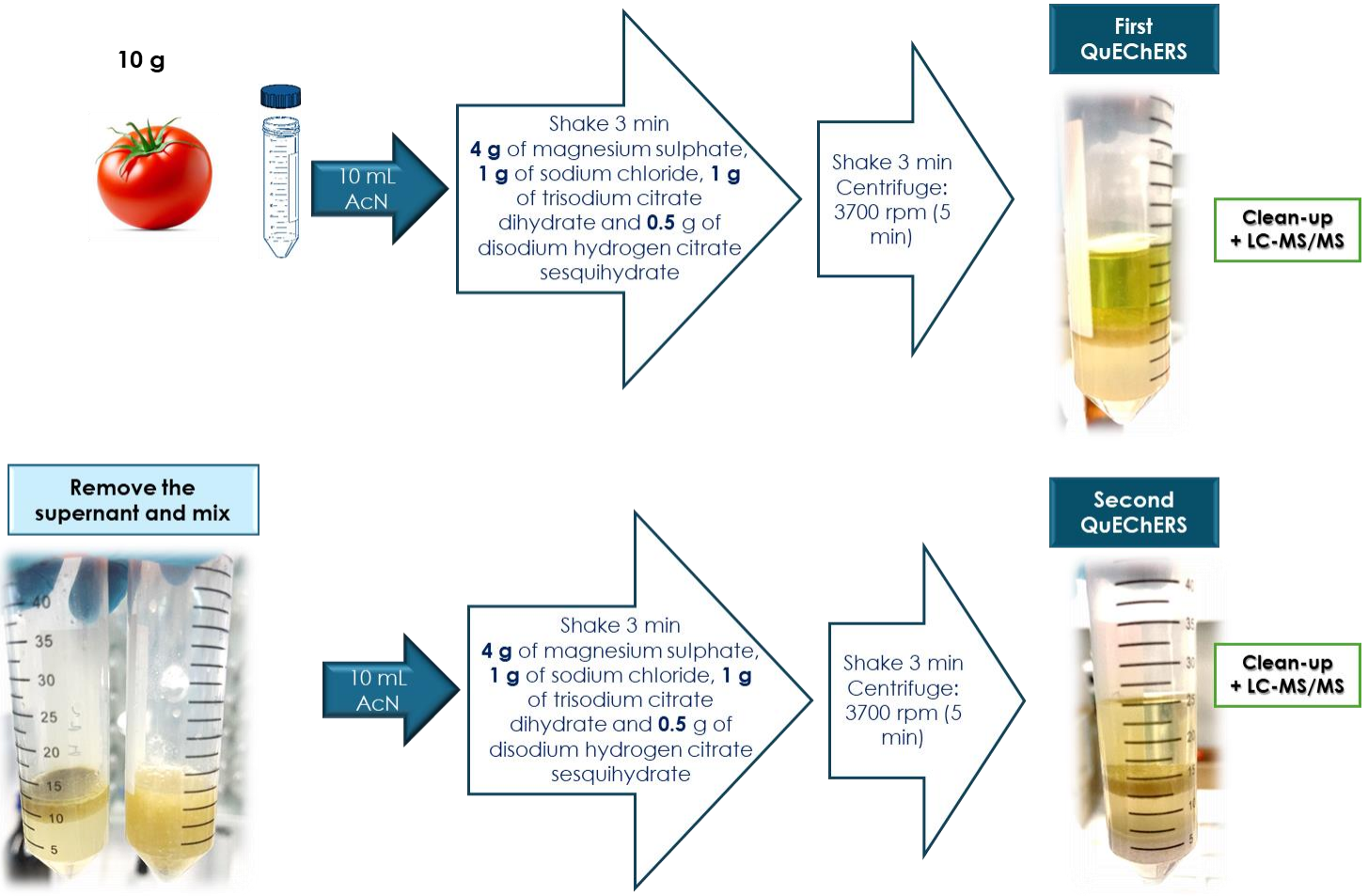

Figure 1: Scheme of the evaluated procedure

For quantification, a matrix-matched calibration curve (0.005, 0.010, 0.020, 0.100, 0.200 and 0.300 mg/kg) was prepared in the following way. First, calibration points in acetonitrile at the indicated concentrations were prepared. Then, 400 µL of Optima® water (with dimethoate-d6 as injection standard), 100 µL of blank sample and 50 µL of standard in acetonitrile were added to all injection vials. For sample vials, pure acetonitrile was added instead of adding the standard.

3.2. Analysis by LC-QqQ-MS/MS

All samples were analyzed by LC operating in multiple reaction monitoring mode (MRM). Selected reaction monitoring (SRM) experiments were carried out to obtain the maximum sensitivity for the detection of the target molecules. For confirmation of the studied compounds, two SRM transitions and a correct ratio between the abundances of the two optimised SRM transitions (SRM2/SRM1) were used, along with retention time matching. The mass transitions used are presented in **Appendix I (Table 1).**

Instrumentation and analytical conditions for the LC- MS/MS system

- Column: Zorbax Eclipse Plus C8 2.1x100 mm and 1.8 µm particle size
- Mobile phase A: Water (0.1 % formic acid, 5 mM ammonium formate, 2 % MeOH)
- Mobile phase B: Methanol (0.1 % formic acid, 5 mM ammonium formate, 2 % water)
- Column temperature: 35 °C
- Flow rate: 0.3 ml/min
- Injection volume: 5 µL
- Autosampler temperature: 12 °C

Mobile phase gradient for pesticides analysis (**Figure 2**):

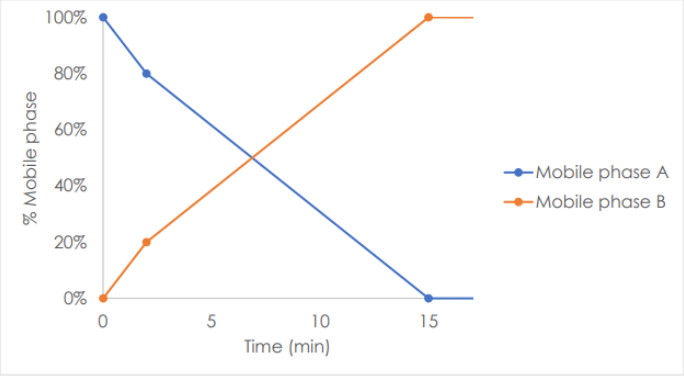

Figure 2: Elution gradient of LC-MS/MS method. Mobile phase gradient used. A (Water (0.1 % formic acid, 5 mM ammonium formate, 2 % MeOH)) and B (Methanol (0.1 % formic acid, 5 mM ammonium formate, 2 % water))

Triple quadrupole system

- Ionisation mode: Positive and negative

- Capillary (positive and negative): 3000 V
- Nebulizer: 45 psi
- Nozzel: 400 V
- Drying gas flow: 13 L/min
- Drying gas temperature: 120 °C
- Sheat gas flow: 10 L/min
- Sheat gas temperature: 375 °C
- High Pressure RF (Positive): 150 V
- High Pressure RF (Negative):110 V
- Low Pressure RF (Positive): 60 V
- Low Pressure RF (Negative): 60 V

4. Results and discussion

4.1. Consecutive QuEChERS extractions

4.1.1 Tomato samples

Table 1 shows the concentrations expressed in µg/kg for the positives in tomato samples. Additionally, the percentage representing the concentration of the second extraction relative to the concentration of the first extraction is calculated.

Table 1: Concentrations in µg/kg obtained in first and second treatment and relative %

Tomato

Sample 1	**First Treatment**	**Second treatment**	**relative %**
Acetamiprid	17.0	0.8	**5**
Propamocarb	78.0	8.5	**11**
Sample 2	**First Treatment**	**Second treatment**	**%**
Acetamiprid	20.0	0.9	**5**
Flonicamid	11.0	0.5	**5**
Fluopyram	7.0	0.0	**0**
Flupyradifurone	41.0	2.1	**5**
Pyrimethanil	20.0	2.3	**12**
Tebufenpyrad	10.0	2.6	**26**
Sample 3	**First Treatment**	**Second treatment**	**%**
Pyriproxyfen	186.0	55.7	**30**
Sample 4	**First Treatment**	**Second treatment**	**%**
Fluopyram	4.5	0.0	**0**
Pyriproxyfen	36.0	4.9	**14**

An example is propamocarb in sample 1; in **Figure 2**, the transitions obtained after the first extraction are shown at the top, and those after the second extraction are shown at the bottom.

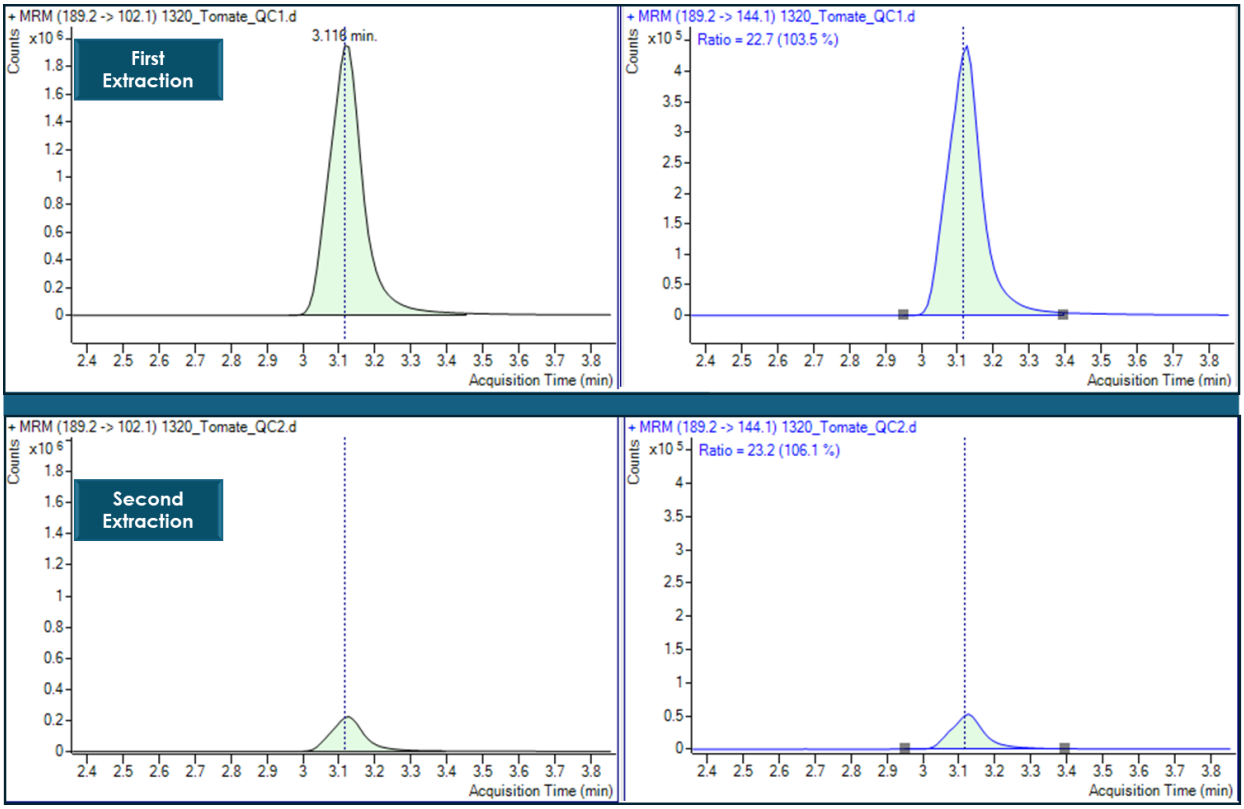

Figure 2: Propamocarb in tomato sample 1 comparative between first extraction and second extraction.

4.1.2 Spinach samples

Table 2 shows the concentrations expressed in µg/kg for the positives in spinach samples. Additionally, the percentage representing the concentration of the second extraction relative to the concentration of the first extraction is calculated.

Table 2: Concentrations in µg/kg obtained in first and second treatment and relative %

Spinach

Sample 1	**First Treatment**	**Second treatment**	**relative %**
Chlorantraniliprole	272.5	22.4	**8**
Mandipropamid	272.5	21.7	**8**
Propamocarb	1182.5	185.8	**16**
Sample 2	**First Treatment**	**Second treatment**	**%**
Chlorantraniliprole	376.0	56.0	**15**
Mandipropamid	1100.0	164.0	**15**
Sample 3	**First Treatment**	**Second treatment**	**%**
Chlorantraniliprole	442.0	44.0	**10**
Mandipropamid	1134.0	132.0	**12**
Propamocarb	15850.0	2920.0	**18**

4.1.3 Banana samples

Table 3 shows the concentrations expressed in µg/kg for the positives in banana samples. Additionally, the percentage representing the concentration of the second extraction relative to the concentration of the first extraction is calculated.

Table 3: Concentrations in µg/kg obtained in first and second treatment and relative %

Banana

Sample 1	**First Treatment**	**Second treatment**	**relative %**
Acetamiprid	16.3	2.9	**18**
Azoxystrobin	454	18.2	**4**
Sample 2	**First Treatment**	**Second treatment**	**%**
Acetamiprid	78.7	14.9	**19**
Azoxystrobin	1438	75.2	**5**
Sample 3	**First Treatment**	**Second treatment**	**%**
Azoxystrobin	164	7.7	**5**
Pyriproxyfen	174.8	15.4	**9**
Sample 4	**First Treatment**	**Second treatment**	**%**
Azoxystrobin	221.1	11.1	**5**

Sample 5	First Treatment	Second treatment	%
Azoxystrobin	19.2	0.2	**1**

4.1.4 Strawberry samples

Table 4 shows the concentrations expressed in µg/kg for the positives in strawberry samples. Additionally, the percentage representing the concentration of the second extraction relative to the concentration of the first extraction is calculated.

Table 4: Concentrations in µg/kg obtained in first and second treatment and relative %

Strawberry			
Sample 1	**First Treatment**	**Second treatment**	**% relative**
Clofentezine	206.3	17.7	**9**
Fluopyram	1530.0	223.3	**15**
Trifloxystrobin	1288.0	154.8	**12**
Sample 2	**First Treatment**	**Second treatment**	**%**
Avermectin B1a	12.9	0.0	**0**
Bupirimate	16.6	2.5	**15**
Difenoconazole	23.5	2.3	**10**
Fluopyram	31.0	0.0	**0**
Fluxapyroxad	50.2	2.2	**4**
Trifloxystrobin	21.6	0.0	**0**

4.1.5. Zucchini samples

Table 5 shows the concentrations expressed in µg/kg for the positives in zucchini samples. Additionally, the percentage representing the concentration of the second extraction relative to the concentration of the first extraction is calculated.

Table 5: Concentrations in µg/kg obtained in first and second treatment and relative %

Zucchini			
Sample 1	**First Treatment**	**Second treatment**	**% relative**
Fluopyram	55.0	1.9	**3**
Flupyradifurone	8.2	0.1	**1**

Propamocarb	88.6	13.4	**15**
Sample 2	**First Treatment**	**Second treatment**	**%**
Difenoconazole	12.2	1.0	**8**
Sample 3	**First Treatment**	**Second treatment**	**%**
Flonicamid	20	0.7	**4**
Fluopyram	113.6	5.2	**5**
Sample 4	**First Treatment**	**Second treatment**	**%**
Acetamiprid	10.8	0.0	**0**
Fluopyram	10.0	0.0	**0**
Propamocarb	121.8	19.5	**16**

4.1.6. Melon samples

Table 6 shows the concentrations expressed in µg/kg for the positives in melon samples. Additionally, the percentage representing the concentration of the second extraction relative to the concentration of the first extraction is calculated.

Table 6: Concentrations in µg/kg obtained in first and second treatment and relative %

Melon

Sample 1	**First Treatment**	**Second treatment**	**% relative**
Fluopyram	114.8	9	**8**
Sample 2	**First Treatment**	**Second treatment**	**%**
Propamocarb	11.0	1.4	**13**
Sample 3	**First Treatment**	**Second treatment**	**%**
Fluopyram	117.7	8.2	**7**
Sample 4	**First Treatment**	**Second treatment**	**%**
Fluopyram	71.8	5.0	**7**

4.2. Extraction time

For the evaluation of extraction time, two samples were selected: tomato and strawberry. The shaking times evaluated were 3, 6, and 10 minutes. (**Figure 3**). The detected pesticides were quantified using matrix-matched calibration curves with a blank that had undergone the same extraction method.

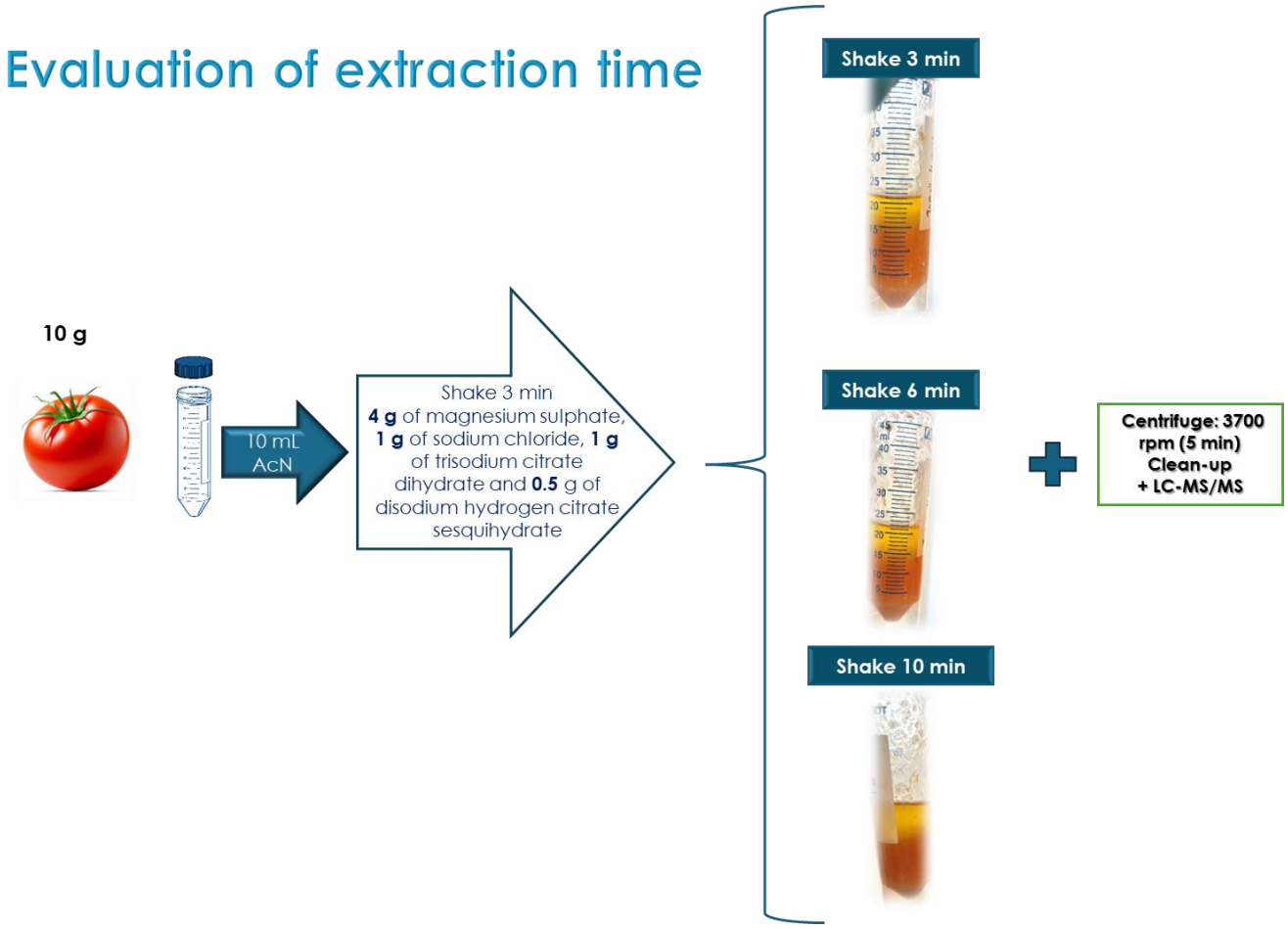

Figure 3: Scheme of the evaluation of the extraction times assessed.

Table 7 presents the results for the evaluated samples. It can be observed that there are no significant differences, as the concentrations obtained are similar at 3 minutes, 6 minutes, and 10 minutes of agitation.

Table 7: Pesticide concentrations expressed in µg/kg at extraction times with QuEChERS salts: 3, 6 or 10 min.

	Tomato		
Sample 2	**3min**	**6 min**	**10 min**
Acetamiprid	20.0	18.6	20.0
Flonicamid	11.0	10.0	10.5
Fluopyram	7.0	5.8	6.4
Flupyradifurone	41.0	37.9	39.4
Pyrimethanil	20.0	16.7	18.0
Tebufenpyrad	10.0	9.9	10.7

Strawberry			
Sample 2	**3min**	**6 min**	**10 min**
Avermectin B1a	12.9	12.9	11.2
Bupirimate	13.1	10.1	11.3
Difenoconazole	19.6	18.7	19.1
Fluopyram	31.0	30.4	29.9
Fluxapyroxad	50.2	47.9	48.7
Trifloxystrobin	21.6	20.3	21.2

5. Conclusions

The study investigates the effectiveness of the QuEChERS method in extracting incurred pesticide residues from various crop samples, including tomatoes, spinaches, bananas, strawberries, zucchinis, and melons. Unlike spiked samples, incurred residues are integrated into the plant tissues, reflecting more realistic conditions of pesticide use in agriculture, such as irrigation and spraying.

The results show that a single extraction does not fully capture the pesticide residues, as seen in the variable recovery rates across different matrices. In the second extraction, a significant reduction in pesticide concentration was observed, indicating that some residues remain bound within the plant tissues despite the initial extraction. Tomato samples, for instance, had a 10% average relative concentration in the second treatment, while spinach had 13%, highlighting the impact of crop type on extraction efficiency (**Table 8**).

Table 8: Average of relative % of concentration extracted in the second treatment

Matrix	***Tomato***	***Spinach***	***Banana***	***Strawberry***	***Zucchini***	***Melon***
% Average	10	13	8	7	6	9

On the other hand, no significant differences were observed at agitation times of 3, 6, and 10 minutes when using QuEChERS citrate salts, suggesting that shorter agitation times may be sufficient under these conditions for the studied matrices.

APPENDIX I: MASS TRANSITIONS AND VALIDATION RESULTS

Table 1. Detection and chromatographic parameters for the compounds analyzed by LC-MS/MS.

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Acephate	184	143	2.816	380	5	Positive
Acephate	184	125	2.816	380	15	Positive
Acetamiprid	223	126	6.041	380	20	Positive
Acetamiprid	223	56	6.041	380	15	Positive
Alachlor	270.1	238.1	11.865	380	10	Positive
Alachlor	270.1	162	11.865	380	20	Positive
Albendazole	266.2	234.1	10.104	380	15	Positive
Albendazole	266.2	191	10.104	380	20	Positive
Aldicarb-sulfone	239.9	223	3.653	380	5	Positive
Aldicarb-sulfone	239.9	86	3.653	380	20	Positive
Ametoctradin	276.2	176.1	12.991	380	35	Positive
Ametoctradin	276.2	149	12.991	380	35	Positive
Anilofos	368.1	198.7	12.521	380	10	Positive
Anilofos	368.1	170.9	12.521	380	20	Positive
Atrazine	216.2	173.8	9.766	380	15	Positive
Atrazine	216.2	131.9	9.766	380	20	Positive
Azinphos-ethyl	368	160.1	11.63	380	10	Positive
Azinphos-ethyl	368	131.9	11.63	380	15	Positive
Azinphos-methyl	318	261	10.364	380	0	Positive
Azinphos-methyl	318	132.1	10.364	380	8	Positive
Azoxystrobin	404	372	10.749	380	10	Positive
Azoxystrobin	404	344	10.749	380	20	Positive
BAC 10	276.2	184.3	11.446	380	20	Positive
BAC 10	276.2	90.8	11.446	380	25	Positive
BAC 8	248.3	156.2	9.792	380	15	Positive
BAC 8	248.3	91.2	9.792	380	35	Positive
Benalaxyl	326.2	208	12.579	380	15	Positive
Benalaxyl	326.2	148	12.579	380	15	Positive
Bendiocarb	224.1	166.7	8.717	380	5	Positive
Bendiocarb	224.1	109.1	8.717	380	20	Positive
Benzovindiflupyr	398	377.9	12.483	380	10	Positive
Benzovindiflupyr	398	342	12.483	380	15	Positive
Bifenazate	301.1	198.2	11.567	380	10	Positive
Bifenazate	301.1	169.9	11.567	380	20	Positive
Bifenazate-diazene	299.2	213.2	12.865	380	5	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Bifenazate-diazene	299.2	183.9	12.865	380	26	Positive
Bitertanol	338.2	269.2	12.711	380	5	Positive
Bitertanol	338.2	99.1	12.711	380	10	Positive
Boscalid	343	307.1	11.057	380	16	Positive
Boscalid	343	272.1	11.057	380	32	Positive
Bromacil	261	204.8	8.606	380	25	Negative
Bromacil	261	81.1	8.606	380	25	Negative
Bromuconazole	378	159	11.827	380	20	Positive
Bromuconazole	378	70	11.827	380	20	Positive
Bupirimate	317	272	11.739	380	20	Positive
Bupirimate	317	166	11.739	380	20	Positive
Buprofezin	306	201	13.649	380	10	Positive
Buprofezin	306	116	13.649	380	15	Positive
Butoxycarboxim	240.1	222.7	3.595	380	5	Positive
Butoxycarboxim	240.1	165.9	3.595	380	5	Positive
Carbaryl	202	145	9.027	380	10	Positive
Carbaryl	202	127	9.027	380	20	Positive
Carbendazim	192	160	4.166	380	15	Positive
Carbendazim	192	132	4.166	380	20	Positive
Carbendazim-D3	195.1	159.8	4.155	380	20	Positive
Carbendazim-D3	195.1	131.9	4.155	380	20	Positive
Carbofuran	222	165	8.717	380	10	Positive
Carbofuran	222	123	8.717	380	15	Positive
Chlorantraniliprole	483.9	452.9	10.415	380	16	Positive
Chlorantraniliprole	483.9	285.9	10.415	380	8	Positive
Chlorbromuron	292.9	203.9	11.002	380	20	Positive
Chlorbromuron	292.9	181.9	11.002	380	15	Positive
Chlorfenvinphos	358.9	155	12.78	380	8	Positive
Chlorfenvinphos	358.9	99.2	12.78	380	28	Positive
Chlorfluazuron	540	382.9	14.307	380	20	Positive
Chlorfluazuron	540	158.1	14.307	380	15	Positive
Chloridazon	222.1	104.1	5.978	380	20	Positive
Chloridazon	222.1	92	5.978	380	20	Positive
Chlorotoluron	213.1	140	9.512	380	20	Positive
Chlorotoluron	213.1	72	9.512	380	20	Positive
Chloroxuron	291.2	217.8	11.476	380	20	Positive
Chloroxuron	291.2	71.9	11.476	380	20	Positive
Chlorpyrifos	352	200	13.791	380	20	Positive
Chlorpyrifos	349.93	198	13.791	380	20	Positive
Chlorpyrifos-methyl	321.9	289.9	12.86	380	14	Positive
Chlorpyrifos-methyl	321.9	125	12.86	380	16	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Chromafenozide	395.2	339.1	11.873	380	5	Positive
Chromafenozide	395.2	174.9	11.873	380	10	Positive
Clofentezine	303	138	12.48	380	12	Positive
Clofentezine	303	102	12.48	380	40	Positive
Clomazone	240.1	127.8	10.544	380	10	Positive
Clomazone	240.1	124.9	10.544	380	20	Positive
Coumaphos	363	307	12.366	380	20	Positive
Coumaphos	363	227	12.366	380	28	Positive
Cyantraniliprole	474.9	444	9.259	380	15	Positive
Cyantraniliprole	474.9	285.8	9.259	380	25	Positive
Cyazofamid	325	261.2	11.915	380	10	Positive
Cyazofamid	325	108.1	11.915	380	15	Positive
Cyflufenamid	413	294.9	12.892	380	15	Positive
Cyflufenamid	413	240.8	12.892	380	15	Positive
Cyhalofop-butyl	375.1	256	13.119	380	15	Positive
Cyhalofop-butyl	375.1	120.1	13.119	380	15	Positive
Cymoxanil	199.1	128	6.437	380	4	Positive
Cymoxanil	199.1	110.9	6.437	380	12	Positive
Cyproconazole	292.1	125	11.52	380	32	Positive
Cyproconazole	292.1	70	11.52	380	16	Positive
Cyprodinil	226.2	92.9	11.666	380	40	Positive
Cyprodinil	226.2	76.9	11.666	380	40	Positive
DEET	192.1	119	10.042	380	15	Positive
DEET	192.1	91.1	10.042	380	20	Positive
Deltamethrin	522.9	280.8	14.505	380	10	Positive
Deltamethrin	520.9	278.7	14.505	380	10	Positive
Demeton-S-methyl	230.9	89.1	8.764	380	5	Positive
Demeton-S-methyl	230.9	61.1	8.764	380	20	Positive
Demeton-S-methylsulfone	263.02	169	4.401	380	12	Positive
Demeton-S-methylsulfone	263.02	109	4.401	380	24	Positive
Demeton-S-methylsulfoxide (Oxydemeton-methyl)	247	169	4.131	380	8	Positive
Demeton-S-methylsulfoxide (Oxydemeton-methyl)	247	109	4.131	380	24	Positive
Desethylterbuthylazine	202.1	146.1	9.06	380	15	Positive
Desethylterbuthylazine	202.1	110.1	9.06	380	20	Positive
Diazinon	305	169	12.598	380	15	Positive
Diazinon	305	153	12.598	380	20	Positive
Dichlorvos	220.8	108.8	8.563	380	15	Positive
Dichlorvos	220.8	78.9	8.563	380	30	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Dichlorvos-D6	226.9	132.9	8.511	380	20	Positive
Dichlorvos-D6	226.9	115	8.511	380	20	Positive
Dicrotophos	238.09	112.1	5.154	380	8	Positive
Dicrotophos	238.09	72.1	5.154	380	28	Positive
Diethofencarb	268	226	10.703	380	5	Positive
Diethofencarb	268	180	10.703	380	15	Positive
Difenoconazole	406	337	12.936	380	15	Positive
Difenoconazole	406	251	12.936	380	20	Positive
Difenoxuron	287.2	123.1	9.939	380	15	Positive
Difenoxuron	287.2	72.1	9.939	380	15	Positive
Diflubenzuron	311	158	11.941	380	8	Positive
Diflubenzuron	311	141	11.941	380	32	Positive
Dimethoate	230	199	6.065	380	5	Positive
Dimethoate	230	171	6.065	380	10	Positive
Dimethoate-D6	236	205	6	380	4	Positive
Dimethoate-D6	236	131	6	380	16	Positive
Dimethomorph	388	301	11	380	20	Positive
Dimethomorph	388	165	11	380	20	Positive
Dimethylvinphos	331	204.8	11.56	380	10	Positive
Dimethylvinphos	331	127	11.56	380	10	Positive
Diniconazole	326.1	159	13.049	380	28	Positive
Diniconazole	326.1	70	13.049	380	28	Positive
Dinotefuran	203.1	129.1	3.28	380	9	Positive
Dinotefuran	203.1	114.1	3.28	380	9	Positive
Diuron	233.03	160	10.092	380	20	Positive
Diuron	233.03	72.1	10.092	380	20	Positive
Diuron	233.03	46.1	10.092	380	16	Positive
DMA	122	106.9	6.357	380	15	Positive
DMA	122	79.1	6.357	380	20	Positive
DMA	122	77.1	6.357	380	20	Positive
Dodine	228.2	60.1	12.617	380	20	Positive
Dodine	228.2	57.2	12.617	380	20	Positive
Edifenphos	311.1	282.8	12.401	380	10	Positive
Edifenphos	311.1	110.9	12.401	380	20	Positive
Emamectin B1a benzoate	886.5	302.2	13.456	380	35	Positive
Emamectin B1a benzoate	886.5	158.1	13.456	380	40	Positive
EPN	324.05	296.01	12.974	380	10	Positive
EPN	324.05	156.99	12.974	380	20	Positive
Epoxiconazole	330.1	121	11.804	380	16	Positive
Epoxiconazole	330.1	101.2	11.804	380	52	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Ethiofencarb	226.1	163.8	9.392	380	5	Positive
Ethiofencarb	226.1	107.2	9.392	380	10	Positive
Ethion	385.1	199	13.8	380	5	Positive
Ethion	385.1	171	13.8	380	10	Positive
Ethiprole	397	351	11.055	380	20	Positive
Ethiprole	397	254.8	11.055	380	40	Positive
Ethirimol	210.16	140.1	7.351	380	20	Positive
Ethirimol	210.16	43.1	7.351	380	52	Positive
Ethoprophos	243.1	130.9	11.905	380	15	Positive
Ethoprophos	243.1	97	11.905	380	30	Positive
Etofenprox	394.2	359.1	14.98	380	10	Positive
Etofenprox	394.2	177.3	14.98	380	8	Positive
Etoxazole	360	304	14.114	380	20	Positive
Etoxazole	360	140.9	14.114	380	30	Positive
Famoxadone	392	331	12.536	380	10	Positive
Famoxadone	392	238	12.536	380	20	Positive
Fenamidone	312	92.2	11.056	380	28	Positive
Fenamidone	312	65.1	11.056	380	56	Positive
Fenamiphos	304.1	234	12.121	380	12	Positive
Fenamiphos	304.1	217.1	12.121	380	20	Positive
Fenamiphos-sulfone	336.1	266	9.029	380	16	Positive
Fenamiphos-sulfone	336.1	188	9.029	380	24	Positive
Fenamiphos-sulfoxide	320.11	292.1	8.808	380	8	Positive
Fenamiphos-sulfoxide	320.11	108.1	8.808	380	44	Positive
Fenarimol	331	268	11.788	380	20	Positive
Fenarimol	331	259	11.788	380	20	Positive
Fenazaquin	307.3	161.3	14.419	380	15	Positive
Fenazaquin	307.3	147.2	14.419	380	15	Positive
Fenbendazole	300.1	268	11.196	380	20	Positive
Fenbendazole	300.1	158.9	11.196	380	35	Positive
Fenbuconazole	337.1	125.1	11.97	380	40	Positive
Fenbuconazole	337.1	70	11.97	380	33	Positive
Fenhexamid	302	97	11.698	380	25	Positive
Fenhexamid	302	55	11.698	380	30	Positive
Fenobucarb	208.2	151.9	10.882	380	5	Positive
Fenobucarb	208.2	95.1	10.882	380	20	Positive
Fenoxycarb	302.2	116.2	12.073	380	5	Positive
Fenoxycarb	302.2	88.2	12.073	380	20	Positive
Fenpicoxamid	615.3	515	13.348	380	13	Positive
Fenpicoxamid	615.3	238.9	13.348	380	25	Positive
Fenpropathrin	367.2	350	14.273	380	5	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Fenpropathrin	367.2	124.8	14.273	380	15	Positive
Fenpropidin	274.3	147.1	10.38	380	30	Positive
Fenpropidin	274.3	85.8	10.38	380	25	Positive
Fenpropimorph	304.3	147.1	10.661	380	30	Positive
Fenpropimorph	304.3	130	10.661	380	25	Positive
Fenpyrazamine	332.2	272.1	11.553	380	10	Positive
Fenpyrazamine	332.2	230.2	11.553	380	20	Positive
Fenpyroximate	422.21	366.2	13.97	380	12	Positive
Fenpyroximate	422.21	107	13.97	380	64	Positive
Fensulfothion	309	252.8	10.009	380	17	Positive
Fensulfothion	309	157	10.009	380	29	Positive
Fenthion	279	247.1	12.326	380	8	Positive
Fenthion	279	169.1	12.326	380	12	Positive
Fenthion-sulfone	310.7	125	9.286	380	15	Positive
Fenthion-sulfone	310.7	108.8	9.286	380	15	Positive
Fenthion-sulfoxide	295.02	280	8.986	380	16	Positive
Fenthion-sulfoxide	295.02	109	8.986	380	32	Positive
Fenuron	165.2	92.1	5.674	380	20	Positive
Fenuron	165.2	71.8	5.674	380	20	Positive
Fipronil	434.9	329.9	12.28	380	12	Negative
Fipronil	434.9	249.9	12.28	380	28	Negative
Flazasulfuron	408	227	10.457	380	20	Positive
Flazasulfuron	408	182.1	10.457	380	20	Positive
Flonicamid	230.1	202.6	4.38	380	10	Positive
Flonicamid	230.1	173.9	4.38	380	10	Positive
Florpyrauxifen-benzyl	441.2	90.9	12.781	380	55	Positive
Florpyrauxifen-benzyl	439.2	91.1	12.781	380	40	Positive
Fluacrypyrim	427.1	205	13.118	380	10	Positive
Fluacrypyrim	427.1	145.1	13.118	380	15	Positive
Fluazifop	328.2	282.2	10.969	380	15	Positive
Fluazifop	328.2	254.2	10.969	380	20	Positive
Flubendiamide	680.9	273.9	12.457	380	15	Negative
Flubendiamide	680.9	254	12.457	380	20	Negative
Fludioxonil	265.9	228.9	11.131	380	5	Positive
Fludioxonil	265.9	158	11.131	380	20	Positive
Flufenacet	364.1	194.1	11.912	380	15	Positive
Flufenacet	364.1	152	11.912	380	15	Positive
Flufenoxuron	489.1	158	14.07	380	20	Positive
Flufenoxuron	489.1	140.9	14.07	380	56	Positive
Fluometuron	233.2	187.9	9.461	380	20	Positive
Fluometuron	233.2	72.2	9.461	380	20	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Fluopicolide	382.9	172.9	11.329	380	20	Positive
Fluopicolide	382.9	144.8	11.329	380	20	Positive
Fluopyram	397.1	208	11.765	380	20	Positive
Fluopyram	397.1	173.1	11.765	380	20	Positive
Flupyradifuron	289.2	126	6.13	380	20	Positive
Flupyradifuron	289.2	72.9	6.13	380	75	Positive
Fluquinconazole	376	307.1	11.55	380	24	Positive
Fluquinconazole	376	108	11.55	380	56	Positive
Flusilazole	316.1	247.1	12.159	380	12	Positive
Flusilazole	316.1	165	12.159	380	24	Positive
Flutriafol	302.1	95	9.897	380	56	Positive
Flutriafol	302.1	70.1	9.897	380	16	Positive
Fluxapyroxad	381.9	362	11.302	380	10	Positive
Fluxapyroxad	381.9	342	11.302	380	15	Positive
Forchlorfenuron	248	128.9	9.948	380	20	Positive
Forchlorfenuron	248	93	9.948	380	30	Positive
Formetanate Hydrochloride	222.13	165.1	2.89	380	8	Positive
Formetanate Hydrochloride	222.13	65.1	2.89	380	52	Positive
Fosthiazate	284	227.8	9.52	380	10	Positive
Fosthiazate	284	103.8	9.52	380	20	Positive
Haloxyfop	362.1	316.2	12.22	380	12	Positive
Haloxyfop	362.1	288.1	12.22	380	24	Positive
Haloxyfop-methyl	375.9	316	13.076	380	15	Positive
Haloxyfop-methyl	375.9	287.9	13.076	380	25	Positive
Hexaconazole	314.1	159	12.775	380	30	Positive
Hexaconazole	314.1	70.1	12.775	380	20	Positive
Hexaflumuron	459	439	13.121	380	5	Negative
Hexaflumuron	459	276.1	13.121	380	20	Negative
Hexythiazox	353.1	228.2	13.98	380	10	Positive
Hexythiazox	353.1	168.2	13.98	380	20	Positive
Imazalil	297	255	9.508	380	15	Positive
Imazalil	297	159	9.508	380	20	Positive
Imidacloprid	256	209	5.287	380	15	Positive
Imidacloprid	256	175	5.287	380	15	Positive
Indoxacarb	528.1	218	13.131	380	20	Positive
Indoxacarb	528.1	203	13.131	380	45	Positive
Ioxynil	369.8	214.8	10.096	380	30	Negative
Ioxynil	369.8	126.8	10.096	380	30	Negative
Iprovalicarb	321.2	202.9	11.883	380	0	Positive
Iprovalicarb	321.2	119	11.883	380	16	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Isofenfos-methyl	231	199	12.39	380	15	Positive
Isofenfos-methyl	231	121	12.39	380	15	Positive
Isoprocarb	194.1	152	9.917	380	5	Positive
Isoprocarb	194.1	95.1	9.917	380	15	Positive
Isoprothiolane	291	230.7	11.248	380	10	Positive
Isoprothiolane	291	189.1	11.248	380	15	Positive
Isoproturon	207.15	165.1	9.984	380	20	Positive
Isoproturon	207.15	72.1	9.984	380	10	Positive
Isopyrazam	360.214	320	9	380	29	Positive
Isopyrazam	360.214	244	9	380	31	Positive
Isoxaflutole	360	250.9	10.168	380	15	Positive
Isoxaflutole	360	219.7	10.168	380	50	Positive
Kresoxim-methyl	314.1	267	12.26	380	0	Positive
Kresoxim-methyl	314.1	222.1	12.26	380	10	Positive
Linuron	249.02	160.1	10.784	380	20	Positive
Linuron	249.02	133	10.784	380	36	Positive
Lufenuron	508.9	339	13.742	380	10	Negative
Lufenuron	508.9	325.9	13.742	380	10	Negative
Malathion	331	285	11.283	380	5	Positive
Malathion	331	127.1	11.283	380	15	Positive
Malathion-D10	341.11	132	11.315	380	12	Positive
Malathion-D10	341.11	100	11.315	380	24	Positive
Mandipropamid	412.13	356.1	11.153	380	4	Positive
Mandipropamid	412.13	328.1	11.153	380	8	Positive
Mebendazole	296.1	263.9	9.227	380	21	Positive
Mebendazole	296.1	105	9.227	380	37	Positive
Mebendazole	296.1	77	9.227	380	55	Positive
Metaflumizone	505	328	13.377	380	10	Negative
Metaflumizone	505	302	13.377	380	10	Negative
Metalaxyl	280.3	220	10.103	380	5	Positive
Metalaxyl	280.3	192.4	10.103	380	10	Positive
Metamitron	203.2	174.9	5.662	380	15	Positive
Metamitron	203.2	104.1	5.662	380	15	Positive
Metazachlor	280	212	9	380	25	Positive
Metazachlor	278	213.7	9	380	25	Positive
Metconazole	320.1	125	12.728	380	48	Positive
Metconazole	320.1	70.1	12.728	380	24	Positive
Methamidophos	142.1	125	2.305	380	10	Positive
Methamidophos	142.1	94.1	2.305	380	10	Positive
Methidathion	302.9	145	10.294	380	0	Positive
Methidathion	302.9	85.1	10.294	380	15	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Methiocarb	226.1	121.1	10.961	380	12	Positive
Methiocarb	226	169	10.961	380	5	Positive
Methiocarb-sulfone	275	201.1	6.353	380	5	Positive
Methiocarb-sulfone	275	122	6.353	380	15	Positive
Methiocarb-sulfoxide	242	185	5.792	380	10	Positive
Methiocarb-sulfoxide	242	170	5.792	380	20	Positive
Methomyl	163.1	106	4.114	380	4	Positive
Methomyl	163.1	88	4.114	380	0	Positive
Methoxyfenozide	369.3	149	11.567	380	15	Positive
Methoxyfenozide	369.3	133	11.567	380	20	Positive
Metobromuron	259	170	9.576	380	15	Positive
Metobromuron	259	148	9.576	380	10	Positive
Metolachlor	284.2	252.1	12.013	380	15	Positive
Metolachlor	284.2	175.9	12.013	380	20	Positive
Metrafenone	409.1	226.9	12.83	380	16	Positive
Metrafenone	409.1	209.1	12.83	380	8	Positive
Monocrotophos	224.2	193.1	4.725	380	5	Positive
Monocrotophos	224.2	127	4.725	380	10	Positive
Monolinuron	215.06	148.1	9.175	380	8	Positive
Monolinuron	215.06	126	9.175	380	16	Positive
Monuron	199.1	125.8	8.197	380	20	Positive
Monuron	199.1	71.9	8.197	380	15	Positive
Myclobutanil	289.2	125.1	11.522	380	20	Positive
Myclobutanil	289.2	70.2	11.522	380	15	Positive
Neburon	275.1	113.9	12.294	380	10	Positive
Neburon	275.07	88.1	12.294	380	12	Positive
Neburon	275.07	57.1	12.294	380	20	Positive
Nitenpyram	271	225	3.833	380	10	Positive
Nitenpyram	271	99	3.833	380	10	Positive
Novaluron	490.8	470.7	13.29	380	5	Negative
Novaluron	490.8	305.1	13.29	380	15	Negative
Omethoate	214.1	183	3.118	380	5	Positive
Omethoate	214.1	125	3.118	380	20	Positive
Orthosulfamuron	425	226.9	10.03	380	15	Positive
Orthosulfamuron	425	199.1	10.03	380	15	Positive
Oxadiargyl	341.05	222.9	12.735	380	13	Positive
Oxadiargyl	341.05	150.9	12.735	380	33	Positive
Oxadixyl	279.1	219.2	7.8	380	5	Positive
Oxadixyl	279.1	132.3	7.8	380	32	Positive
Oxamyl	237	90	3.821	380	5	Positive
Oxamyl	237	72	3.821	380	10	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Oxasulfuron	407.1	209.7	8.143	380	24	Positive
Oxasulfuron	407.1	150.1	8.143	380	16	Positive
Oxathiapipronil	540.2	522	11.217	380	29	Positive
Oxathiapipronil	540.2	500	11.217	380	29	Positive
Oxfendazole	316.1	284.1	7.979	380	20	Positive
Oxfendazole	316.1	159.1	7.979	380	35	Positive
Paclobutrazol	294.1	125.2	11.322	380	36	Positive
Paclobutrazol	294.1	70.1	11.322	380	16	Positive
Penconazole	284	159	12.435	380	20	Positive
Penconazole	284	70	12.435	380	15	Positive
Pencycuron	329.1	125.1	12.972	380	24	Positive
Pencycuron	329.1	89.1	12.972	380	60	Positive
Pendimethalin	282.1	212.1	13.889	380	4	Positive
Pendimethalin	282.1	194.1	13.889	380	16	Positive
Penflufen	318.1	234	12.369	380	10	Positive
Penflufen	318.1	141	12.369	380	20	Positive
Penthiopyrad	357.9	207.6	12.538	380	20	Negative
Penthiopyrad	357.9	149	12.538	380	25	Negative
Phenthoate	321	247.1	12.29	380	4	Positive
Phenthoate	321	79.1	12.29	380	44	Positive
Phosalone	368	182	12.739	380	8	Positive
Phosalone	368	110.9	12.739	380	44	Positive
Phosmet	317.99	160	10.458	380	8	Positive
Phosmet	317.99	133	10.458	380	36	Positive
Phoxim	299	129.1	12.668	380	4	Positive
Phoxim	299	77.1	12.668	380	24	Positive
Pirimicarb	239.2	182.1	7.618	380	15	Positive
Pirimicarb	239.2	72.2	7.618	380	20	Positive
Pirimicarb-desmethyl	225.1	168.1	5.26	380	8	Positive
Pirimicarb-desmethyl	225.1	72.1	5.26	380	20	Positive
Pirimiphos-methyl	306.2	164.2	12.664	380	20	Positive
Pirimiphos-methyl	306.2	108.2	12.664	380	20	Positive
Prochloraz	376	308	12.493	380	10	Positive
Prochloraz	376	266	12.493	380	15	Positive
Profenofos	374.9	347	13.417	380	5	Positive
Profenofos	374.9	304.9	13.417	380	15	Positive
Promecarb	208.2	150.9	11.247	380	5	Positive
Promecarb	208.2	108.8	11.247	380	10	Positive
Prometryn	242.2	201	11.033	380	20	Positive
Prometryn	242.2	157.8	11.033	380	20	Positive
Propamocarb	189.2	144.1	3.271	380	10	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Propamocarb	189.2	102.1	3.271	380	15	Positive
Propaquizafop	444.1	371	13.454	380	15	Positive
Propaquizafop	444.1	99.9	13.454	380	20	Positive
Propargite	368.1	231.2	14.126	380	0	Positive
Propargite	368.1	175.2	14.126	380	8	Positive
Propazine	230.2	187.9	10.868	380	15	Positive
Propazine	230.2	146	10.868	380	20	Positive
Propiconazole	342.1	159	12.48	380	32	Positive
Propiconazole	342.1	69.1	12.48	380	16	Positive
Propoxur	210.11	168.1	8.595	380	5	Positive
Propoxur	210.11	111.1	8.595	380	10	Positive
Propyzamide	256	190	11.31	380	10	Positive
Propyzamide	256	173	11.31	380	20	Positive
Proquinazid	373	331	14.152	380	20	Positive
Proquinazid	373	289.1	14.152	380	20	Positive
Prosulfocarb	252.1	128	13.319	380	10	Positive
Prosulfocarb	252.1	90.9	13.319	380	20	Positive
Prothioconazole	341.9	99.8	12.603	380	20	Negative
Prothioconazole	341.9	306.1	12.603	380	15	Negative
Pyraclostrobin	388.11	193.8	12.536	380	8	Positive
Pyraclostrobin	388.11	163.1	12.536	380	20	Positive
Pyridaben	365.2	309.2	14.536	380	10	Positive
Pyridaben	365.2	147.3	14.536	380	20	Positive
Pyridalyl	490	203.9	15.324	380	20	Positive
Pyridalyl	490	108.8	15.324	380	20	Positive
Pyridaphenthion	341.1	205	11.502	380	20	Positive
Pyridaphenthion	341.1	189	11.502	380	15	Positive
Pyridate	379.1	351.1	14.782	380	5	Positive
Pyridate	379.1	206.8	14.782	380	10	Positive
Pyrimethanil	200	183	10.068	380	20	Positive
Pyrimethanil	200	107	10.068	380	20	Positive
Pyriofenone	366.1	209	12.863	380	20	Positive
Pyriofenone	366.1	183.9	12.863	380	20	Positive
Pyriproxyfen	322	185	13.633	380	20	Positive
Pyriproxyfen	322	96	13.633	380	10	Positive
Quinalphos	299.1	270.8	12.122	380	10	Positive
Quinalphos	299.1	242.8	12.122	380	10	Positive
Quinoclamine	208	105.1	7.697	380	25	Positive
Quinoclamine	208	77	7.697	380	40	Positive
Quinoxyfen	308.1	271.9	13.705	380	25	Positive
Quinoxyfen	308.1	196.9	13.705	380	35	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Quizalofop	345	299	11.834	380	20	Positive
Quizalofop	345	254.9	11.834	380	35	Positive
Quizalofop-ethyl	373.09	271.2	13.254	380	24	Positive
Quizalofop-ethyl	373.09	255.1	13.254	380	36	Positive
Rotenone	395	213.1	11.894	380	20	Positive
Rotenone	395	192.1	11.894	380	20	Positive
Simazine	202.2	131.8	8.447	380	15	Positive
Simazine	202.2	124	8.447	380	15	Positive
Spinetoram J	748.3	203	13.075	380	30	Positive
Spinetoram J	748.3	142	13.075	380	25	Positive
Spinetoram L	760.4	203	13.393	380	35	Positive
Spinetoram L	760.4	142.1	13.393	380	35	Positive
Spinosyn A	732.5	142.1	12.589	380	30	Positive
Spinosyn A	732.5	98.1	12.589	380	40	Positive
Spinosyn D	746.5	142	12.95	380	25	Positive
Spinosyn D	746.5	98	12.95	380	40	Positive
Spirodiclofen	411.1	313	14.429	380	5	Positive
Spirodiclofen	411.1	71.2	14.429	380	15	Positive
Spiromesifen	371	273	14.218	380	5	Positive
Spiromesifen	371	255	14.218	380	20	Positive
Spirotetramat	374.2	330.3	11.723	380	15	Positive
Spirotetramat	374.2	270.1	11.723	380	20	Positive
Spiroxamine	298	144	11.015	380	20	Positive
Spiroxamine	298	100	11.015	380	20	Positive
Sulfoxaflor	278	153.9	6.49	380	20	Positive
Sulfoxaflor	278	105.1	6.49	380	10	Positive
Tau-fluvalinate	503	208	14.792	380	20	Positive
Tau-fluvalinate	503	181.1	14.792	380	20	Positive
Tebuconazole	308	125	12.448	380	20	Positive
Tebuconazole	308	70	12.448	380	20	Positive
Tebufenozide	353.2	296.9	12.345	380	5	Positive
Tebufenozide	353.2	133.1	12.345	380	15	Positive
Tebufenpyrad	334.2	145.1	13.576	380	20	Positive
Tebufenpyrad	334.2	117	13.576	380	47	Positive
Teflubenzuron	379	359	13.573	380	0	Negative
Teflubenzuron	379	339	13.573	380	4	Negative
Terbutryn	242.2	186.2	11.146	380	15	Positive
Terbutryn	242.2	91	11.146	380	20	Positive
Terbutylazine	230	174	11.065	380	15	Positive
Terbutylazine	230	146	11.065	380	20	Positive
Tetraconazole	372	159	11.921	380	36	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Tetraconazole	372	70	11.921	380	20	Positive
Tetramethrin	332.1	163.9	13.47	380	15	Positive
Tetramethrin	332.1	135.1	13.47	380	15	Positive
Thiabendazole	202	175	4.83	380	30	Positive
Thiabendazole	202	131	4.83	380	40	Positive
Thiacloprid	253	186	6.754	380	10	Positive
Thiacloprid	253	126	6.754	380	20	Positive
Thiamethoxam	292	211	4.378	380	10	Positive
Thiamethoxam	292	181	4.378	380	20	Positive
Thiobencarb	258	124.7	12.824	380	15	Positive
Thiobencarb	258	99.9	12.824	380	10	Positive
Tolclofos-methyl	300.9	269	12.621	380	10	Positive
Tolclofos-methyl	300.9	125	12.621	380	15	Positive
Tolfenpyrad	384.1	197	13.534	380	25	Positive
Tolfenpyrad	384.1	170.9	13.534	380	20	Positive
Triadimefon	294.2	225	11.475	380	10	Positive
Triadimefon	294.2	197.1	11.475	380	10	Positive
Triadimenol	296	227	11.4	380	5	Positive
Triadimenol	296	70	11.4	380	10	Positive
Triallate	306.01	145	13.935	380	25	Positive
Triallate	306.01	86	13.935	380	15	Positive
Triazophos	314.1	286.2	11.523	380	10	Positive
Triazophos	314.1	162.2	11.523	380	20	Positive
Trichlorfon	258.9	222.5	5.961	380	5	Positive
Trichlorfon	258.9	108.8	5.961	380	20	Positive
Triclorcarban	313	160	13.103	380	20	Negative
Triclorcarban	313	126	13.103	380	20	Negative
Tricyclazole	190.1	163	7.025	380	25	Positive
Tricyclazole	190.1	136.1	7.025	380	35	Positive
Trifloxystrobin	409.2	206.2	13.199	380	10	Positive
Trifloxystrobin	409.2	186.2	13.199	380	20	Positive
Triflumizole	346.1	277.8	13.234	380	5	Positive
Triflumizole	346.1	72.9	13.234	380	15	Positive
Triflumuron	359	156	12.709	380	8	Positive
Triflumuron	359	139	12.709	380	32	Positive
Trinexapac-ethyl	253.1	68.9	10.158	380	20	Positive
Trinexapac-ethyl	253.1	41.1	10.158	380	45	Positive
Trinexapac-methyl	239.1	69	9.076	380	10	Positive
Trinexapac-methyl	239.1	41.2	9.076	380	40	Positive
Triticonazole	318.1	125.2	11.785	380	20	Positive
Triticonazole	318.1	70.2	11.785	380	20	Positive

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Ret Time (min)	Fragmentor (V)	Collision Energy (eV)	Polarity
Tritosulfuron	446	195	10.607	380	20	Positive
Tritosulfuron	446	145	10.607	380	40	Positive
Valifenalate	399	313	11.58	380	10	Positive
Valifenalate	399	143.7	11.58	380	15	Positive
XMC	180.1	123.1	9.04	380	10	Positive
XMC	180.1	95.1	9.04	380	20	Positive
Zoxamide	336	187	12.594	380	16	Positive
Zoxamide	336	159	12.594	380	44	Positive